WE CLAIM:

1. A method of identifying components of a mixture, said method comprising the steps of:

obtaining a set of spectral data for a mixture, the set of spectral data defining a mixture data space;

ranking a plurality of library spectra of known elements according to their angle of projection into the mixture data space;

calculating a corrected correlation coefficient for each combination of the top *y* ranked library spectra; and

selecting the combination having the highest corrected correlation coefficient, wherein the known elements of the selected combination are identified as the components of the mixture.

2. The method of claim 1, wherein the plurality of library spectra of known elements are ranked using target factor testing techniques.

3. The method of claim 1, wherein the step of calculating a corrected correlation coefficient for each combination of the top *y* ranked library spectra comprises the steps of:

calculating a correlation coefficient for each known element included in a given combination;

combining the correlation coefficients for the known elements included in the given combination to develop a cumulative correlation coefficient value;

developing cumulative eigenvalues for the given combination; and

multiplying the cumulative correlation coefficient value by the cumulative eigenvalues to develop the corrected correlation coefficient for the given combination.

4. The method of claim 3, wherein the step of combining the correlation coefficients comprises the step of calculating the square root of the sum of the squares of the correlation coefficients for the known elements included in the given combination to develop the cumulative correlation coefficient for the given combination.

5. The method of claim 3, wherein the step of combining the correlation coefficients comprises the step of calculating the square root of the sum of the squares of the correlation coefficients for the known elements included in the given combination divided by the number of known elements included in the given combination to develop the cumulative correlation coefficient for the given combination.

6. The method of claim 3, wherein the step of calculating a correlation coefficient comprises the steps of:

calculating a projected library spectrum for each known element included in the given combination; and

measuring the similarity of the projected library spectrum with its actual library spectrum to develop the correlation coefficient for each known element in the given combination.

7. The method of claim 6, wherein the step of measuring the similarity of the projected library spectrum with its actual library spectrum comprises the steps of:

calculating the dot product of the projected library spectrum with the actual library spectrum; and

dividing the calculated dot product by the multiplication of the dot product of the projected library spectrum with itself and the dot product of the actual library spectrum with itself to develop the correlation coefficient for each known element in the given combination.

8. The method of claim 6, wherein the step of calculating a projected library spectrum comprises the steps of:

using the obtained mixture spectra and the known library spectra to calculate relative concentrations of each known element included in the given combination; and

using the calculated relative concentrations and the obtained mixture spectra to calculate the projected library spectrum for each known element included in the given combination.

9. The method of claim 8, wherein if any known element in the given combination is calculated to have a negative relative concentration, eliminating the given combination from consideration.

10. The method of claim 8, wherein if any known element in the given combination is calculated to have a negative relative concentration:

calculating the ratio of a maximum positive calculated relative concentration for the given combination to the average of the sum of the absolute values of the calculated negative relative concentrations for the given combination; and

if the calculated ratio is less than a predetermined number, eliminating the given combination from consideration.

11. The method of claim 8, wherein if any known element in the given combination is calculated to have a negative relative concentration:

calculating the ratio of a maximum positive calculated relative concentration for the given combination to the average of the sum of the absolute values of the calculated negative relative concentrations divided by the number of concentrations that are negative for the given combination; and

if the calculated ratio is less than a predetermined number, eliminating the given combination from consideration.

12. The method of claim 11, wherein the predetermined number comprises 4.0.

13. The method of claim 1, wherein y is equal to 10.

14. The method of claim 1, where the plurality of library spectra of known elements are ranked according to their angle of projection into the mixture data space, from smallest to largest.

15. The method of claim 1, further comprising the step of correcting the set of spectral data to remove signals and information not due to the chemical composition of the mixture.

16. The method of claim 1, further comprising the steps of:

obtaining, at a later point in time, another set of spectral data for the mixture, such that the another set of spectral data is separated from the set of spectral data by a time interval, the another set of spectral data defining another mixture data space;

ranking a plurality of library spectra of known elements according to their angle of projection into the another mixture data space;

calculating a corrected correlation coefficient for each combination of the top *y* ranked library spectra; and

selecting the combination having the highest corrected correlation coefficient, wherein the known elements of the selected combination are identified as the components of the mixture at the later point in time.

17. The method of claim 16, further comprising the step of using the identified components of the mixture from both the set of spectral data and the another set of spectral data to analyze trends in the composition of the mixture over the time interval.

18. The method of claim 1, wherein the set of spectral data comprises a plurality of spectral data sets obtained from the mixture at different points in time.

19. The method of claim 1, wherein the set of spectral data comprises a plurality of spectral data sets obtained from the mixture at different locations in the mixture.

20. A method of identifying components of a mixture from a set of spectral data obtained from the mixture and defining a mixture data space, said method comprising the steps of:

ranking, based on the set of spectral data, a plurality of library spectra of known elements according to their likelihood of being a component of the mixture, from most likely to least likely;

calculating a ranking criterion for each combination of the top *y* ranked library spectra; and

selecting a combination based on the ranking criterion, wherein the known elements of the selected combination are identified as the components of the mixture.

21. The method of claim 20, where the plurality of library spectra are ranked according to their angle of projection into the mixture data space.

22. The method of claim 20, wherein the ranking criterion comprises a corrected correlation coefficient, and wherein the step of selecting a combination based on the ranking criterion comprises the step of selecting the combination having the highest corrected correlation coefficient, wherein the known elements of the selected combination are identified as the components of the mixture.

23. The method of claim 22, wherein the step of calculating a corrected correlation coefficient for each combination of the top *y* ranked library spectra comprises the steps of:

calculating a correlation coefficient for each known element included in a given combination;

combining the correlation coefficients for the known elements included in the given combination to develop a cumulative correlation coefficient value;

squaring the cumulative correlation coefficient value;

developing cumulative eigenvalues for the given combination; and

multiplying the squared cumulative correlation coefficient value by the cumulative eigenvalues to develop the corrected correlation coefficient for the given combination.

24. The method of claim 23, wherein the step of calculating a correlation coefficient comprises the steps of:

calculating a projected library spectrum for each known element included in the given combination; and

measuring the similarity of the projected library spectrum with its actual library spectrum to develop the correlation coefficient for each known element in the given combination.

25. The method of claim 24, wherein the step of calculating a projected library spectrum comprises the steps of:

using the obtained mixture spectra and the known library spectra to calculate relative concentrations of each known element included in the given combination; and

using the calculated relative concentrations and the obtained mixture spectra to calculate the projected library spectrum for each known element included in the given combination,

wherein if any known element in the given combination is calculated to have a negative relative concentration:

calculating the ratio of a maximum positive calculated relative concentration for the given combination to the average of the sum of the absolute values of the calculated negative relative concentrations divided by the number of concentrations that are negative for the given combination; and

if the calculated ratio is less than a predetermined number, eliminating the given combination from consideration.

26. The method of claim 20, further comprising the steps of:

obtaining, at a later point in time, another set of spectral data from the mixture, such that the another set of spectral data is separated from the set of spectral data by a time interval, the another set of spectral data defining another mixture data space;

ranking, based on the another set of spectral data, a plurality of library spectral of known elements according to their likelihood of being a component of the mixture, from most likely to least likely;

calculating a ranking criterion for each combination of the top *y* ranked library spectra; and

selecting a combination based on the ranking criterion, wherein the known elements of the selected combination are identified as the components of the mixture at the later point in time.

27. The method of claim 26, further comprising the step of using the identified components of the mixture from both the set of spectral data and the another set of spectral data to analyze trends in the composition of the mixture over the time interval.

28. The method of claim 26, wherein the ranking criterion comprises a corrected correlation coefficient, and wherein the step of selecting a combination

based on the ranking criterion comprises the step of selecting the combination having the highest corrected correlation coefficient, wherein the known elements of the selected combination are identified as the components of the mixture.

29. The method of claim 20, further comprising the steps of:

obtaining another set of spectral data from the mixture at a location different from a location of the set of spectral data, the another set of spectral data defining another mixture data space;

ranking, based on the another set of spectral data, a plurality of library spectral of known elements according to their likelihood of being a component of the mixture, from most likely to least likely;

calculating a ranking criterion for each combination of the top *y* ranked library spectra; and

selecting a combination based on the ranking criterion, wherein the known elements of the selected combination are identified as the components of the mixture at the different location.

30. The method of claim 29, further comprising the step of using the identified components of the mixture from both the set of spectral data and the another set of spectral data to analyze trends in the composition of the mixture over its spatial area.

based on the ranking criterion comprises the step of selecting the combination having the highest corrected correlation coefficient, wherein the known elements of the selected combination are identified as the components of the mixture.

29. The method of claim 20, further comprising the steps of:

obtaining another set of spectral data from the mixture at a location different from a location of the set of spectral data, the another set of spectral data defining another mixture data space;

ranking, based on the another set of spectral data, a plurality of library spectral of known elements according to their likelihood of being a component of the mixture, from most likely to least likely;

calculating a ranking criterion for each combination of the top *y* ranked library spectra; and

selecting a combination based on the ranking criterion, wherein the known elements of the selected combination are identified as the components of the mixture at the different location.

30. The method of claim 29, further comprising the step of using the identified components of the mixture from both the set of spectral data and the another set of spectral data to analyze trends in the composition of the mixture over its spatial area.